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Structures and electronic transport in nanoelectronic devices based on carbon nanotube complexes.

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Abstract. The geometrical structure of and electron transport in carbon nanotube complexes are studied. A general method to construct theoretically three-tube unions for nanotubes of different types is developed. Then study electron packet evolution in obtained structures using semiempirical tight-binding model in π -electron approximation.

Introduction

Carbon nanotubes-tubulenes, discovered in 1991 by Iijima [1], are molecular cylindrical surfaces which are close-packed with atomic carbon hexagons and are obtained by the thermal decomposition of graphite. They can be represented geometrically as the result of gluing a strip cut from a single graphite plane. Normally nanotubes are classified by two indexes i_1 and i_2 , those define nanotube chirality and radii. Depending on the indexes, a set of atomic carbon structures with a wide spectrum of conducting properties is obtained — from semiconductors with gap widths of 0–2 eV to semimetals, of which graphite is a typical representative [2].

Using this fact, many authors have thought [3] that nanodiodes could be studied theoretically and then can be manufactured. This nanodiodes can be made of two carbon nanotubes of different indexes and different electronic band structure. Now there are some calculations about the conductivity of these structures [4], and there are also works with experimental data about point defects in nanotubes, but by now there are only a few number of them.

We think that the next step could be investigating nanotransistors, and it is possible to imagine that they can be constructed by joining three tubes at the same end. Each one of this tubes may be equivalent to the different semiconductor type in a standard NPN transistor. In our situation, we can have two identical tubes (N zones) and another one with different chirality and band structure (P zone).

1 Geometrical structure of the three-tubed connection

We have developed a general method to construct theoretically this kind of three-tube unions in an easy way. Our structure will consist now in three tubes joined by a union (from now, the union) where we must place six heptagons, as the Euler's theorem says, but we don't know where. At least, we know that an heptagon placed inside a graphitic lattice produces a negative curvature in this surface, like in the schwarzites, and the points of the union with this kind of curvature are between the beginning of each pair of tubes. That is the reason why we can assume that the heptagons will be near this points.

Now, if we want to know if every union with 6 heptagons can lead to a global structure with three tubes, we must center our attention in the position of the heptagons near the points of negative curvature. We can always connect them by paths consisting of a certain number of carbonated rings, which can be pentagons, hexagons or heptagons. We may think that in our three-tubed structure we can connect the six heptagons by three paths (strips made of rings) glued at their ends, so each tube is held by two strips.

As an example, in a knee tube (tube that presents a curved aspect, but it is really a pair of tubes with different chirality joined one each other) the structure has one strip connecting the pentagon and the heptagon (as in this structures we have the same number of heptagons and pentagons) which leads to both tubes.

But we can make ourselves this question: How can this strip lead to two tubes? If we fix both ends of the strip, we will obtain a tube-like structure, to which we may only add hexagons to verify if a cylinder can appear. That is the same technic we already know to form a normal nanotube (we take a vector and superpose the two hexagons at the start and end of the vector) but it is more general. For example, in a strip made only of hexagons, we can superpose the two hexagons in the end of the strip in six different ways, by rotating one hexagon over another. It is clear that if we do this with only hexagons we will never obtain a tube, but a cone. But if we have heptagons or pentagons maybe it will be useful.

Now, if we are going to study the different effects produced by heptagons and pentagons in these strips, we need to arrive to this conclusion: When we add hexagons next to the strips we must obtain tubes, and that is the reason why if we follow by continuity the orientation of the added hexagons, its change must be 0.

So, if we locate an heptagon or a pentagon in the strip, we can do it in two different ways, 'up' and 'down', that means that the strip is curved upwards or downwards, respectively. We always fixed two arbitrary orientations at the end and at the beginning of the strip. For simplicity we take a specified one and we do it this way: We draw a path of hexagons, and we mark two parallel orientations at the end and the beginning of the strip. Then we substitute some of the hexagons by pentagons and heptagons in positions 'up' or 'down'.

Within these specifications, it is easy to observe that the heptagon in the position 'up' induces a turn of 0 and in the position 'down', a turn of 60° .

Directly we can do the same with pentagons in positions 'up' and 'down', which produces turns of -60 in the position 'up' and 0 in the position 'down'.

If we closed our strip the way we showed before, to obtain over and below the union two tubes, we need that the rotation induced becomes 0. It must be no a multiple of 360, because this produces a different topology structure, like a plane, or a fulleren cup. We will return to this discussion later in our work. We can now write two equations that the structure must verify to lead to two tubes. Let $h_a, h_{a'}$ the number of heptagons that produces a turn of 60 in the side a , and in a' , and $p_a, p_{a'}$ the number of pentagons that produces a turn of -60 in both sides.

$$60(h_a - p_a) = 0$$

$$-60(h_{a'} - p_{a'}) = 0.$$

The conclusion is obvious: we must have the same number of pentagons and heptagons. We need this only for training to afford the construction of a union to glue three tubes.

With three tubes, the tubes will be formed by two strips, so we must take account of this in our equations. We must also be careful with the connections of each pair of strips, because in everyone there is a change of the references' orientation.

When we go from one strip to another, if the references were chosen as we said, we can see that the reference turns an angle of $180 - \alpha$, where α is the angle between strips a and b in the first of the two hexagons that connect the three strips. (The same way β and γ are the angles between b and c , and between c and a . We will denote the angles in the other hexagon with α' , β' and γ' .) This is because the turn of the reference is the angle complementary of α . And if the reference is turned a certain angle, we must subtract this angle to our equations.

These will remain like this:

$$60(h_a - p_a + h_{b'} - p_{b'}) - (180 - \alpha) - (180 - \alpha') = 0$$

$$60(h_b - p_b + h_{c'} - p_{c'}) - (180 - \beta) - (180 - \beta') = 0$$

$$60(h_c - p_c + h_{a'} - p_{a'}) - (180 - \gamma) - (180 - \gamma') = 0.$$

If we use the fact that, if the strips are joined by an hexagon, the sum of the three angles (of each hexagon) is 360, we can conclude this:

$$60(h_A + h_B + h_C - p_A - p_B - p_C) = 360$$

where we denoted with h_A, h_B and h_C the respective sums of h_a and $h_{a'}$, h_b and $h_{b'}$, h_c and $h_{c'}$, that is the total number of pentagons and heptagons in the strips A, B and C. It implies an excess of six heptagons, as we previously knew, but the important fact is that we have found three equations that the union must follow to lead to three tubes.

So, we can vary the position of the heptagons and pentagons in the strips, as the length of the strip in order to obtain different structures. Now we also know the rules we must follow to obtain three tubes. We also here propose a method to denote this kind of structures, describing the strips by its indexes and marking the positions of the pentagons and heptagons in them.

2 Electron transport in nanotube complexes

A characteristic feature of the energy structure of the valence electrons of a single graphite plane is the existence of π -electrons, whose states can be described by a simple analytical model, at Fermi level; σ -electrons at the Fermi-level have an energy gap of the order 10 eV. When a ideal tubulene is glued from a strip cut from a graphite plane, the perturbation of the σ and π -electrons depends on the dimensionless parameter a/R , where a is the distance between the closest atoms in the graphite plane and R is the radius of the tubulene. For the tubulenes with a large radius this perturbation is weak, and accordingly the electronic spectrum of a tubulene can be obtained from that of an isolated graphite plane; this approximation is widely employed in the literature and is termed zone folding [2]. For tubulenes with small radii, the finiteness of the perturbation, which can result hybridisation of the π - and σ -electrons, must be taken into account. However for simplicity we applied π -electron model in present investigation of electron transport in nanotubes and their complexes. The hamiltonian matrix is constructed in semiempirical tight-binding model in nearest-neighbouring approximation.

We have applied before this model to calculate electronic structure and properties of ideal graphitic nanotubes [5].

The quantum state of π -electron in infinite carbon nanotube is classified by two quantum numbers, m — magnetic quantum number and k_z — the electron impulse along the nanotube axis. Electronic state energy depends on nanotube radius, chirality, numbers m and k_z . In the elastic scattering on the nanotube connection the scattering amplitude depends on radii and chiralities of connected tubes. It may be calculated by numerical integration of nonstationary Schrodinger equation. It is necessary to make Gauss electron wave packet with fixed m on the one of the nanotubes. The packet length along the tube depends on dispersion of the impulse k_z . Numerical integrating of Schrödinger equation in tight-binding approximation give us the packet evolution across the nanotube connection, so one may obtain the scattering amplitude. We use the norm-conserving numeric schemes based on Pade-approximation of the evolution operator on the each time step. This method allow us to calculate the electron transport in the complexes described before and in other more complicated structures those can be useful to construct nanodevices.

References

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